

Topological Superconductivity without Proximity Effect

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Majorana Fermions, strange particles that are their own antiparticles, were predicted in 1937 and have been sought after ever since. In condensed matter they are predicted to exist as vortex core or edge excitations in certain exotic superconductors. These are topological superconductors whose order parameter phase winds non-trivially in momentum space. In recent years, a new and promising route for realizing topological superconductors has opened due to advances in the field of topological insulators. Current proposals are based on semiconductor heterostructures, where spin-orbit coupled bands are split by a band gap or Zeeman field and superconductivity is induced by proximity to a conventional superconductor. Topological superconductivity is obtained in the interface layer. The proposed heterostructures typically include two or three layers of different materials. In the current work we propose a device based on materials with inherent spin-orbit coupling and an intrinsic tendency for superconductivity, eliminating the need for a separate superconducting layer. We study a lattice model that includes spin-orbit coupling as well as on-site and nearest neighbor interaction. Within this model we show that topological superconductivity is possible in certain regions of parameter space. These regions of non-trivial topology can be understood as a nodeless superconductor with d-wave symmetry which, due to the spin-orbit coupling, acquires an extra phase twist of 2π .

Back in 1937, Ettore Majorana found particles that arise as real solutions to the Dirac equation. These solutions, called Majorana fermions, partially obey fermionic statistics. While different Majorana fermions anti-commute, each Majorana fermion is its own anti particle. The creation operator of a Majorana fermion is also its annihilation operator or, in other words it is an equal superposition of regular fermionic creation and annihilation operators. This exceptional property captured the imagination of many and the quest to find the Majorana fermion began.

In the context of high energy physics it is speculated that the neutrino might in fact be a Majorana fermion. The testing of this claim, which originated from Majorana himself, has not been possible in the past, as it requires a large collider like the LHC and is still an open question at the time of writing.

Regardless of the nature of the neutrino and possible other elementary particles of the Majorana type, Majorana fermions may be realized in condensed matter systems. In condensed matter, excitations are not limited to elementary particles since they may be emergent particles that are dressed by the medium and interactions in the many body ground state. As such, it is conceivable that emergent excitations be their own anti-particles. Furthermore, in condensed matter anti-particles are provided by holes in energy bands and the superposition of particles and holes is possible. Such a superposition of particles and holes occurs as an excitation in any superconductor, since the number of particles is not conserved due to the presence of a pair condensate.

In order to realize Majorana fermions, a system should exhibit pairing between two particles of the same spin. This requires triplet pairing and particularly a complex p -wave order parameter is desirable. It has been shown[1]

that topological, spin-triplet, $p_x + ip_y$ superconductors will support Majorana fermions in their vortex cores[2]. Some materials have been found to have triplet p -wave pairing; however their topology has yet to be proven to be non-trivial[3]. Therefore, current efforts to realize Majorana fermions have had to focus on devices which lead to quantum states that are either topological superconductors or analogous to them.[1, 4–7] An interesting analogue of a topological superconductor was proposed to describe the fractional quantum Hall state in some fractions[1] and some progress in this direction has been made[8–10]. In that state, Chern-Simons dressed particles minimize their interaction energy by creating a condensate whose symmetry is $p_x + ip_y$. Proving beyond doubt the existence of this state as well as the detection of Majorana fermions therein still remains a challenge.

Recently, inspired by advances in topological insulators, another route to topological superconductivity has opened. Fu and Kane[4] have shown that a three dimensional topological insulator layer placed in proximity to a conventional s -wave superconductor develops topological superconductivity. The pairing in the system is induced by proximity effect while the topology is inherited from the topological insulator. This occurs since the pairing function is projected to one of the spin-orbit coupled bands. In order to accommodate the unique spin structure (and Chern number) of the topological insulator, the induced order parameter must wind its phase by 2π in momentum space.

The idea of Fu and Kane was further developed by Sau *et al.*[5] in the context of semiconductor heterostructures. Sau and coworkers envisioned a semiconductor quantum well with intrinsic Rashba spin-orbit coupling (SOC) where the Fermi surface lies in the band. The required gap between the two spin-orbit coupled bands

is provided by an out of plane Zeeman field of an attached ferromagnetic (FM) insulator layer. Meanwhile, superconductivity is induced by proximity to a superconducting layer attached to the other side of the quantum well.

Recently, Alicea[6] explored the possibility of eliminating the ferromagnetic insulator layer of the Sau *et al* model. Instead of the ferromagnetic insulating layer, Alicea suggested using a quantum well with both Dresselhaus and Rashba SOC while applying an in plane magnetic field. The Dresselhaus SOC tilts the plane in which the electron spins tend to align so that the applied magnetic field can open a gap, eliminating the need for the FM insulator and thereby reducing the complexity of the device.

Another suggestion for the realization of Majorana fermions has been made by Cook and Franz[7]. Their work involves inducing superconductivity in nanotubes and nano-ribbons; the relation between the type of resulting order parameter and symmetries of this model was explored by Fu and Berg[11].

The key aspects of realizing an effective $p + ip$ state in these previous devices has been the proper combination of SOC, band gap or Zeeman splitting and proximity induced pairing. The spin orbit coupling is responsible for the non-trivial spin texture, whereas the Zeeman field (or an intrinsic mass term) splits the bands such that only one of them is relevant at low energy. Meanwhile, the superconductor responsible for inducing pairing through proximity is of a simple singlet type.

In this Letter we use these key ingredients to address the question of whether a topological superconductor can be achieved without proximity effect. In place of proximity induced pairing we consider pairing driven by interactions. Using a variational mean field approach, both phases of trivial and topological superconductivity are found in the model studied. The topological state we find can be described by a superconductor with a 6π phase winding which is a result of the $l = 2$ d-wave phase winding and a $p + ip$ projection function.

In order to test whether interactions may lead to superconductivity in spin-orbit coupled materials we consider a two dimensional square lattice model. The Hamiltonian of the system reads

$$H = H_{KE} + H_{SO} + V, \quad (1)$$

where the kinetic energy term H_{KE} is given by hopping on nearest neighbors.

$$H_{KE} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}). \quad (2)$$

Here t is the hopping amplitude, $\langle i, j \rangle$ are nearest-neighbor lattice sites and σ is a spin index. The spin-orbit coupling part of the Hamiltonian is given by

$$H_{SO} = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger \mathcal{H}_{\mathbf{k}} \psi_{\mathbf{k}}, \quad \mathcal{H}_{\mathbf{k}} = \sigma \cdot \mathbf{d}_{\mathbf{k}} \quad (3)$$

where $\psi_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow})^T$, σ is a 3-vector of Pauli matrices and $\mathbf{d}_{\mathbf{k}} = (A \sin k_x, A \sin k_y, 2B(\cos k_x + \cos k_y - 2) + M)$ with A, B and M material parameters. This term can be viewed as the lattice version of the continuum model introduced by previous authors[4–6] while its form resembles one of the sectors of the model introduced by Bernevig *et al.* to describe HgTe quantum wells[12]. The finite Zeeman splitting M may be the result of a band gap, an external magnetic field or a magnetic field of a near by ferromagnetic layer.

We choose to model the interactions with effective on-site repulsion and nearest neighbor attraction, such as in the extended Hubbard model given by

$$V = U_0 \sum_i n_{i\uparrow} n_{i\downarrow} + V_0 \sum_{\langle i,j \rangle, \sigma, \sigma'} n_{i\sigma} n_{j\sigma'}, \quad (4)$$

with $U_0 > 0$ (repulsion) and $V_0 < 0$ (attraction). The motivation behind introducing an attractive V_0 stems from studies of a similar model without spin-orbit coupling in the context of the cuprates.[13, 14] In the case of the cuprates, it has been shown that on-site repulsion treated in the Eliashberg formalism leads to d -wave pairing on bonds. This same result can be obtained in mean field if one introduces an effective nearest-neighbor attraction as in our model above.

In order to map the phase diagram of the model in Eq. 1 we adopt a variational mean-field theory. Our method involves obtaining a variational wave function that is a solution to an auxiliary quadratic Hamiltonian. This auxiliary Hamiltonian contains the kinetic and spin orbit coupling parts of the Hamiltonian in Eq. 1 as well as a variety of order parameters. These order parameters represent all possible mean field states such as density waves, superconductivity etc. The mean field ground state is found by minimizing the expectation value of the interacting Hamiltonian (*i.e.* Eq. 1) with respect to the parameters of the variational wave function. These parameters are essentially the magnitudes of the various order parameters of the model. The advantage of this method over the usual self-consistent mean-field theory is that it does not assume *a priori* the dominance of any order parameter. More on its application can be found in Reference [15].

To this end, we use the following auxiliary Hamiltonian

$$H_{AUX} = \frac{1}{4} \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \Lambda_{\mathbf{k}} \Psi_{\mathbf{k}} \quad (5)$$

where we have defined the 8-spinor $\Psi_{\mathbf{k}} = (c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}, c_{\mathbf{k}+\mathbf{Q}\uparrow}, c_{\mathbf{k}+\mathbf{Q}\downarrow}, c_{-\mathbf{k}\uparrow}^\dagger, c_{-\mathbf{k}\downarrow}^\dagger, c_{-\mathbf{k}-\mathbf{Q}\uparrow}^\dagger, c_{-\mathbf{k}-\mathbf{Q}\downarrow}^\dagger)^T$ (here $\mathbf{Q} = (\pi, \pi)$) and the matrix

$$\Lambda_{\mathbf{k}} = \begin{pmatrix} h(\mathbf{k}) & \hat{\Delta}(\mathbf{k}) \\ \hat{\Delta}(\mathbf{k})^* & -h(-\mathbf{k})^* \end{pmatrix}, \quad (6)$$

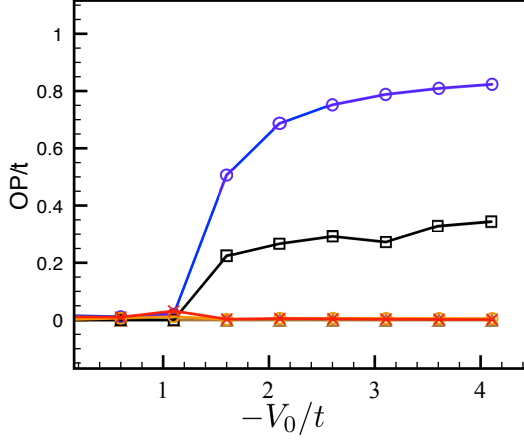


FIG. 1: Sample plot of order parameters. In this figure the magnitude of the order parameters is in units of t and we have fixed $A = 0.25t$, $B = .5t$, $M = .1t$ and $U_0 = 2t$. Circles (blue online) are $\Delta^{(1)}$, squares (black online) are $\Delta^{(2)}$, diamonds (orange online) are $\Delta^{(3)}$, x's (red online), $\Delta^{(4)}$ and triangles (brown online) represent S . This simulation was done on a 100×100 square lattice. The graph shows the development of $d + id$ order since both $\Delta^{(1)}$ and $\Delta^{(2)}$ become non-zero at the critical coupling.

represents the Nambu space of particles and holes. Its entries are 4×4 matrices:

$$h(\mathbf{k}) = \begin{pmatrix} \hat{\mathcal{H}}(\mathbf{k}) & -S\sigma_z \\ -S\sigma_z & \hat{\mathcal{H}}(\mathbf{k} + \mathbf{Q}) \end{pmatrix}, \quad \hat{\mathcal{H}}(\mathbf{k}) = \epsilon_{\mathbf{k}} + \mathcal{H}(\mathbf{k}), \quad (7)$$

and

$$\hat{\Delta}(\mathbf{k}) = i\Delta_{\mathbf{k}}\sigma_y \otimes \tau_z. \quad (8)$$

where $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$ is the tight binding spectrum and $\mathcal{H}_{\mathbf{k}}$ is as defined in Equation (3). In our notation σ_i are Pauli matrices that act on the spin and τ_i are Pauli matrices which denote the sublattice degree of freedom.

In the above auxiliary Hamiltonian we have allowed for the possibility of antiferromagnetism (AF) through the Néel order parameter S , as well as several channels of superconductivity through the order parameter $\Delta_{\mathbf{k}} = \Delta^{(1)}(\cos k_x - \cos k_y) + i\Delta^{(2)}\sin k_x \sin k_y + \Delta^{(3)}(\cos k_x + \cos k_y) + \Delta^{(4)}$. We can now find the variational energy numerically for a given set of order parameters and then minimize with respect to these parameters. This amounts to finding the mean field ground state energy and wave function of the system. A representative plot of these order parameters appears in Fig. 1.

As $\Delta^{(3)} = \Delta^{(4)} = 0$ throughout the plot in Fig. 1, we conclude that this region of parameter space does not support s -wave nor extended s -wave superconductivity. We also see that $S = 0$ in Fig. 1 and so AF is also not a dominant order in this region of parameter space.

The lack of s and extended s -wave superconductivity is a general characteristic of the phase diagram of this model, however depending on how we tune the SOC parameters it is possible to find a state where AF (and not superconductivity) is the dominant ground state.

To demonstrate the differing ground states of our model we present two separate slices of the phase diagram. Figure 2 gives two plots in a space of the interaction parameters V_0 and U_0 ; one slice is for values of A, B and M where the ground state is found to be superconductivity, while the other has the SOC parameters tuned so that we see a phase with an AF ground state. The $d + id$ phase in Fig. 2 is the most interesting for our purposes as it is fully gapped and therefore its topological invariant is well defined. It is obtained when both $\Delta^{(1)}$ and $\Delta^{(2)}$ are non-zero. We view this state as having a projected superconducting order parameter whose phase winds by 6π in momentum space. 4π of the winding is due to its d -wave nature and the remaining 2π are the result of the projection on one of the spin-orbit coupled band. We focus to this $d + id$ region of the phase diagram and investigate the topology of this phase.

Before ending this section, we make a few remarks in passing. First, Fig. 2 showcases a phase that is purely d -wave in nature. One might ask why we are not interested in the topology of this phase; the reason is that this d -wave order parameter has nodes and as a result it is difficult to properly define a topological invariant in this case. Nevertheless, the topology of this superconductor may be an interesting topic for further studies and could be found to be non-trivial. On the other hand, due to nodal excitations any Majorana fermions that may be produced will not be protected against scattering. Second, in the interest of preforming an exhaustive search for competing ground state order in this model, we have checked that neither spin nor charge density waves give a dominant ground state contribution to the model presented here in the studied parameter regime.

To study the topology of the $d + id$ region we calculate the TKNN number[16](equivalent to the first Chern number) using our optimized mean-field wave function. This involves selecting a region in the $d + id$ phase in Fig. 2 and then calculating[17]

$$I = \frac{1}{2\pi} \int d^2k \mathcal{F}(\mathbf{k}) \quad (9)$$

where the Berry curvature, \mathcal{F} , is defined using the eigenstates $\Lambda_{\mathbf{k}}|\phi_n(\mathbf{k})\rangle = E_n(\mathbf{k})|\phi_n(\mathbf{k})\rangle$ viz[18]

$$\mathcal{F}(\mathbf{k}) = i \sum_n' \sum_{m \neq n} \epsilon^{ij} \left[\frac{\langle \phi_n | \frac{\partial \Lambda_{\mathbf{k}}}{\partial k_i} | \phi_m \rangle \langle \phi_m | \frac{\partial \Lambda_{\mathbf{k}}}{\partial k_j} | \phi_n \rangle}{(E_n - E_m)^2} \right], \quad (10)$$

where, for the sake of brevity, we have dropped the functional dependence on \mathbf{k} , the primed sum is a sum over filled bands, the ϵ^{ij} tensor has the values $\epsilon^{1,2} = -\epsilon^{2,1} = 1$

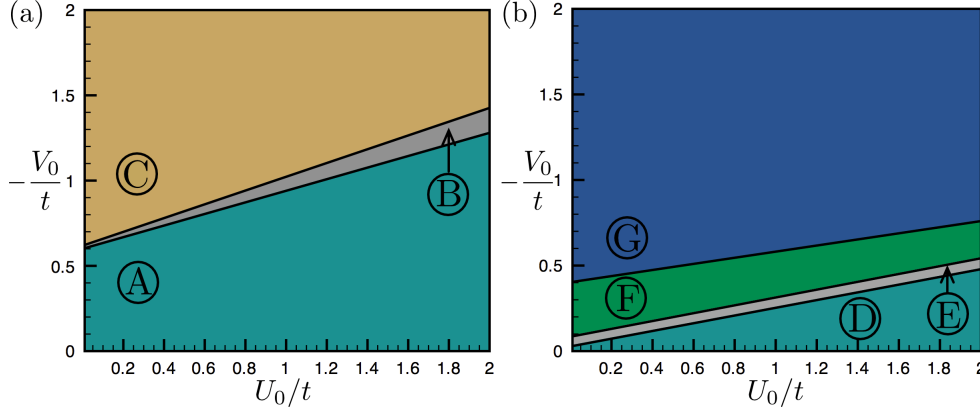


FIG. 2: Slices of the phase diagram. The left plot (plot (a)) showcases a region of parameter space where the ground state of the model is superconductivity. We have set $A = 0.25t$, $B = -0.45t$ and $M = -0.1t$ in this plot. The regions of the phase diagram are labeled A (teal online) for normal (or non-superconducting state), B (grey online) for a d -wave ground state and C (beige online) for $d + id$ superconductivity. The right plot (plot (b)) shows a region of the phase diagram where we can see either antiferromagnetism or superconductivity. Here we have sets $A = 0.25t$, $B = -0.9t$ and $M = -0.05t$ and our labeling is D (teal online) for the normal state, E (grey online) for a d -wave ground state, F (green online) for $d + id$ superconductivity and G (blue online) for AF ground state.

and $\epsilon^{i,i} = 0$ and summation over the repeated indices i and j is implied.

By calculating this invariant we can classify the topology of the $d + id$ region as either trivial (regions for which we find $I = 0$) or non-trivial (regions for which $I = 1$). Our results are summarized in Figure 3. As the topology of the system is intimately related to the number of Fermi surfaces before interactions are turned on[11], Fig. 3 also shows a sample of the Fermi surface in each topological region.

Figure 3 displays one of our main results; our model has regions of $d + id$ topological superconductivity. As an example, Fig. 3 shows that the $d + id$ state in Fig. 2a is topologically trivial while the like in Fig. 2b is topological. Further, we see from the figure some devices might exist in the topologically non-trivial region at some set value of M . It may then be possible to move the system into a topological phase by changing M via either an applied field or proximity to a magnetic layer. In this way, our results suggest that properly applying a Zeeman field (*i.e.* tuning M) to spin-orbit coupled superconductors may result in the transition of an ordinary superconductor to a topological one.

In a real material, it is not possible to tune the interaction. However, this is routinely done in cold atoms. It has been demonstrated recently that spin-orbit coupling may be simulated in cold atoms[19]. This may lead the way for simulating topological insulators[20–22]. Our work suggests that if the spin-orbit coupling and the interactions are tuned correctly, a topological superconductor may be simulated as well.

In summary, we have proposed a model of interacting, spin-orbit coupled, Zeeman split electrons on a square lattice. We have shown that in regions of parameter

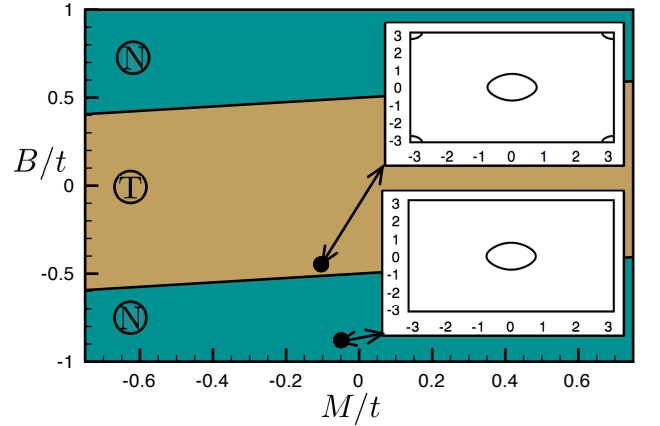


FIG. 3: Topology of the $d + id$ ground state phase. In this figure we have set $A = 0.25t$. The topologically trivial phase is labeled T (beige online) while the non-trivial phase is labeled N (teal online). The insets show an example of the Fermi surface (in the first Brillouin zone) for each phase before interactions are turned on. The lower inset, corresponding to the $d + id$ state of Fig. 2b, shows a single Fermi surface for the topologically non-trivial phase while the upper inset (the $d + id$ state in Fig. 2a) shows two Fermi surfaces in the topologically trivial region.

space the ground state of the proposed model is either a $d + id$ superconductor or an antiferromagnet. Narrowing our focus to the $d + id$ region we have shown that our system supports phases of non-trivial topology. The topological regions in our phase diagrams exhibit superconductivity that exhibits 6π winding of its order parameter phase in the Brillouin zone. In the same way that a $p + ip$ superconductor may support the existence

of Majorana fermions in vortex cores or on edges, this superconductor will support their existence. As our model considers superconductivity driven by interactions rather than the proximity effect, it may serve as a possible simplification for device design. Finally, our work supplies strong evidence that Majorana fermions might be realized in certain spin-orbit coupled superconductors under the proper application of a Zeeman field.

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